

Reconstruction of soft X-ray diffraction patterns – Progress

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Beamline: X1B

Introduction: X-ray diffraction is potentially a strong candidate for biological imaging since it can in principle reconstruct thick samples at resolutions close to the diffraction limit of the radiation. Due to the non-crystalline nature of such samples, one seeks a phasing method other than that of traditional crystallography; such a method exists in the use of an iterative algorithm based on the oversampled diffraction pattern recorded on CCD camera.

Methods and Progress: The diffraction of an object illuminated with coherent X-ray light reveals the Fourier transform of the object's structural and chemical map within the Born approximation. Therefore, the object can be discovered if it is unknown, when the complete diffraction data are available. In reality, the diffraction intensity is recorded and the phase is lost. To handle this, iterative phase recovery based on oversampling has been introduced [1] and successful phase recovery has been reported earlier [1,2,3] using a Fienup-type iterative schema [4]. In our work, the iterative schema of Elser [5] is employed. Figure 1(a) shows the reconstruction of the test sample whose diffraction magnitude is shown in figure 1(b). Though not shown here, the test sample is almost completely recovered in figure 1(a). This simulation shows again the feasibility of iterative phase recovery to reconstruct an unknown object when only diffraction magnitudes are available. In practice, one needs an instrument to record the high resolution diffraction data with the capability of rotating samples for 3D imaging, the ultimate aim of the project. To meet this need, a new instrument has been built by T. Beetz et al. which will be primarily used on the X1B beamline at the NSLS [6]. We have been able to collect the first few diffraction patterns of biological samples (mainly air dried yeast cells) using the new instrument at the NSLS, one of them shown in figure 2. Currently we are investigating the quality of the recorded diffraction patterns and attempts to reconstruct unknown samples using measured diffraction intensities have begun.

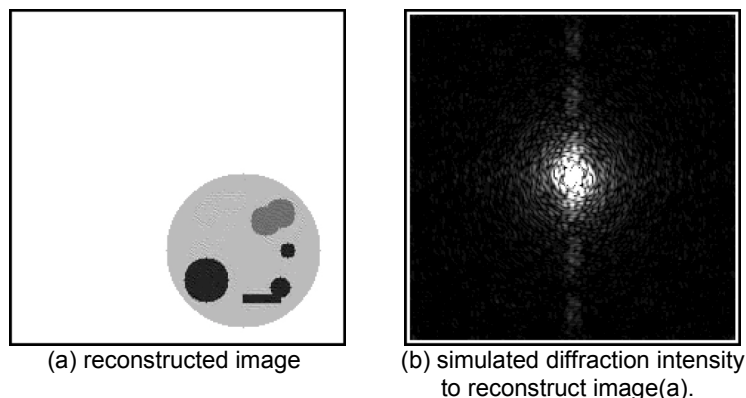


Figure 1. The reconstruction from computer simulation.

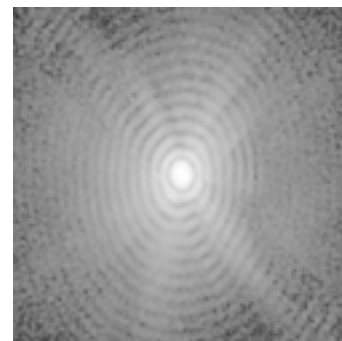


Figure 2. The actual measured diffraction intensity on X1B beamline; high resolution data not shown here.

Acknowledgments: Work is supported in part by NIH grant # NIGMS GM648460 and was performed in part at the NSLS, which is supported by the DOE – BES.

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